Symmetry protected $\mathbb{Z}_2$-quantization and quaternionic Berry connection with Kramers degeneracy

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Abstract. As for a generic parameter dependent hamiltonian with the time reversal (TR) invariance, a non Abelian Berry connection with the Kramers (KR) degeneracy are introduced by using a quaternionic Berry connection. This quaternionic structure naturally extends to the many body system with the KR degeneracy. Its topological structure is explicitly discussed in comparison with the one without the KR degeneracy. Natural dimensions to have non trivial topological structures are discussed by presenting explicit gauge fixing. Minimum models to have accidental degeneracies are given with/without the KR degeneracy, which describe the monopoles of Dirac and Yang. We have shown that the Yang monopole is literally a quaternionic Dirac monopole.

The generic Berry phases with/without the KR degeneracy are introduced by the complex/quaternionic Berry connections. As for the symmetry protected $\mathbb{Z}_2$ quantization of these general Berry phases, a sufficient condition of the $\mathbb{Z}_2$-quantization is given as the inversion/reflection equivalence.

Topological charges of the $SO(3)$ and $SO(5)$ nonlinear σ-models are discussed in their relation to the Chern numbers of the CP^1 and HP^1 models as well.

1. Introduction

Topological numbers have been important in physics especially in quantum phenomena. They give a conceptual foundation of quantizations for various elementary degrees of freedom such as charges, fluxes, vortices and monopoles[1, 2]. One of the milestones of the emerging topological numbers is a quantization of the Hall conductance where a response function is directly related to the topological quantum number as the first Chern number [3, 4, 5, 6, 7]. Its fundamental physical meaning has become clear by introducing an idea of the geometrical concept which is known as the Berry connection today[8]. For the quantum Hall (QH) states, the bulk is gapped and does not have any characteristic symmetry breaking. It results in absent of a local order parameter nor any low energy excitations as the Goldston bosons. A class of such featureless systems is the (gapped) quantum liquid and the spin liquid. A possible effective field theory for the gapped quantum liquids is the topological field theory where topological quantities play a central role. Then corresponding new idea to describe the system is the topological order[9, 10]. It should be compared with the standard Ginzburg-Landau-Wilson scenario, where local field theories to describe fluctuation of a local order parameter is essential. As for a bulk topological ordered state, the degeneracy of the ground state depends on the topology of the physical space[9]. However there were not so much quantities to describe the topological order. As an extension of the success for the QH state, we have successfully used the Berry connections and related topological quantities for characterization of the topological ordered states[11, 12, 13, 14, 15, 16, 17]. Also note that although the bulk QH state is featureless, the system with boundaries has characteristic localized states as the edge states[18, 19]. Extending the observation, we are proposing an idea of the *bulk-edge correspondence*, which says that although the bulk is gapped and only characterized by the topological quantities, there exist characteristic boundary states which reflect the topologically non trivial bulk for the system with boundaries[7, 20]. This "bulk-edge correspondence" seems to be a universal feature of the topological ordered states such as the QH states, quantum spins[13, 21, 17], graphene[22], photonic crystals[23], cold atoms[24], characterization of localizations[25] and quantum spin Hall (QSH) systems[26, 27, 28].

The QSH state is an analogous state to the QH states but it respects the time reversal symmetry by the help of spins[26, 27]. Then it is natural that the Berry connection with the TR invariance play fundamental roles. There have been substantial amount of works for the topic [29, 30, 31, 27, 26, 32, 33, 34, 35, 28, 25, 36, 37, 38, 39]. Here in this paper, we present a self-contained description of the Berry connections and related topological quantities with/without the Kramers (KR) degeneracy. Especially we focus on its quaternioninc structure. The quaternions are fundamental in the description of the TR invariant system with the KR degeneracy which was first pointed out by Dyson long time ago[40, 41, 29, 30]. There is more than an analogy between the system with/without the KR degeneracy. One can make a mapping between them by replacing the complex number by the quaternions[41]. We explicitly demonstrate it for the topological quantities by introducing canonical minimum models, which are related to the monopoles and accidental degeneracies.

As for the topological quantities, there can be two classes. The one includes topological invariants by their definition. The quantization for them is automatically guaranteed only by stability and a regularity of the Berry connections. The examples are the Chern numbers, winding numbers and Pontrjagin index. Additionally we

introduce a new class of quantized quantities as a generalization of the $\mathbb{Z}_2$ Berry phase[13], which is geometrical but as for the quantization, one needs additional symmetry requirement. We give a sufficient condition for this symmetry protected $\mathbb{Z}_2$-quantization.

As for the application of gauge invariant description of the Chern numbers, a relation between the Chern numbers and the topological charges of the $SO(3)$ and $SO(5)$ nonlinear σ-models are also presented shortly.

2. Time reversal and quaternions

Let us first introduce a quaternion notation for a TR invariant bi-linear system[40]. Introducing D parameters $x = (x^1, \cdots, x^\mu, \cdots, x^D) \in V_D$, $\dim V_D = D$, let us consider a bi-linear $2N$-fermion hamiltonian $\mathcal{H}(x) = c_m^\dagger H_{mn}(x) c_n$, $c_n^\dagger = (c_{n\uparrow}^\dagger, c_{n\downarrow}^\dagger)$ where H_{mn} is a 2×2 complex matrix and c_n, $(n = 1, \cdots, N)$ is a spinor, a pair of fermion annihilation operators (summation over doubled indexes is assumed and $n = 1, \cdots, N$). Further let us impose an invariance under the time-reversal (TR) operation Θ for the hamiltonian $\mathcal{H}$. Since Θ operates as $c_{n\sigma} \to (-)^{(\sigma-1)/2} c_{n-\sigma}$ ($\uparrow = +1$ and $\downarrow = -1$, $c_{n\uparrow} \to c_{n\downarrow}$ and $c_{n\downarrow} \to -c_{n\uparrow}$) and taking a complex conjugate $\mathcal{K}$, we have $\tilde{J} H_{mn}^* J = -J H_{mn}^* J = H_{mn}$, $(J = i\sigma_y)$ where $\sigma_{x,y,z}$ are the Pauli matrices ($\tilde{\ }$ is a matrix transpose). As for the bi-linear hamiltonian here, it is expressed as $[H, \Theta_b] = 0$ where $\{H\}_{mn} = H_{mn}$ and $\Theta_b = -\mathcal{K}J$ (J operates sub block of H_{mn}). Now let us expand this 2×2 matrix H_{mn} as $H_{mn} = h_{mn}^0 + h_{mn}^1 I + h_{mn}^2 J + h_{mn}^3 K$ where $I = i\sigma_z = -I^* = -I^\dagger$, $J = i\sigma_y = J^* = -J^\dagger$, $K = i\sigma_x = -K^* = -K^\dagger$. Then the TR invariance implies $h_{mn}^\alpha \in \mathbb{R}$, $(\alpha = 0, \cdots, 3)$, that is, H_{mn} is identified as a quaternion $\mathbb{H} \ni h_{mn}$ by a standard equivalence $I \cong i_{\mathbb{H}}$, $J \cong j_{\mathbb{H}}$, $K \cong k_{\mathbb{H}}$, $i_{\mathbb{H}}, j_{\mathbb{H}}, k_{\mathbb{H}} \in \mathbb{H}$, ${i_{\mathbb{H}}}^2 = {j_{\mathbb{H}}}^2 = {k_{\mathbb{H}}}^2 = i_{\mathbb{H}} j_{\mathbb{H}} k_{\mathbb{H}} = -1$, since $-J H_{mn}^* J = (h_{mn}^0)^*(-JJ) + (h_{mn}^1)^*(-J(-I)J) + (h_{mn}^2)^*(-J(J)J) + (h_{mn}^3)^*(-J(-K)J) \cong (h_{mn}^0)^* + (h_{mn}^1)^* i_{\mathbb{H}} + (h_{mn}^2)^* j_{\mathbb{H}} + (h_{mn}^3)^* k_{\mathbb{H}}$. Hermiticity of the $\mathcal{H}$, $H^\dagger = H$, implies 4 conditions for the *real* matrices, h^α, $\tilde{h}^0 = h^0$, $\tilde{h}^\alpha = -h^\alpha$, $(\alpha = 1, 2, 3)$ where $(h^\alpha)_{mn} \equiv h_{mn}^\alpha$. It gives a hermite quaternionic matrix $h^{\mathbb{H}} = h^0 + h^1 i_{\mathbb{H}} + h^1 i_{\mathbb{H}} + h^2 j_{\mathbb{H}} + h^3 k_{\mathbb{H}} \cong H = h^0 + h^1 I + h^2 J + h^3 K$ expressed as $(h^{\mathbb{H}})^\dagger = h^{\mathbb{H}}$.

As for a normalized eigen state, $\psi_\ell = \begin{bmatrix} \psi_{\ell\uparrow} \\ \psi_{\ell\downarrow} \end{bmatrix}$, $(\psi_\ell^\dagger \psi_\ell = 1)$ of $2N$ dimensional hamiltonian H, $(H\psi_\ell = \epsilon_\ell \psi_\ell)$, it is degenerate with $\psi_\ell^\Theta = \Theta \psi_\ell = \begin{bmatrix} -\psi_{\ell\downarrow}^* \\ \psi_{\ell\uparrow}^* \end{bmatrix}$, which is the Kramers(KR) degeneracy. Its orthogonality, $\psi_\ell^\dagger \psi_\ell^\Theta = 0$, is trivial here (Generically, there are N KR pairs, $\ell = 1, \cdots, N$). Then let us write this KR pair as

$$
\begin{aligned}
\Psi_\ell = (\psi_\ell, \Theta\psi_\ell) &= \psi_\ell^0 \otimes E_2 + \psi_\ell^1 \otimes I + \psi_\ell^2 \otimes J + \psi_\ell^3 \otimes K \\
&= \begin{bmatrix} \psi_\ell^0 + i\psi_\ell^1 & \psi_\ell^2 + i\psi_\ell^3 \\ -\psi_\ell^2 + i\psi_\ell^3 & \psi_\ell^0 - i\psi_\ell^1 \end{bmatrix} \cong \psi_\ell^{\mathbb{H}} \in \mathbb{H}^N,
\end{aligned}
$$

where $\psi_\ell^0 = \mathrm{Re}\,\psi_\ell^\uparrow$, $\psi_\ell^1 = \mathrm{Im}\,\psi_\ell^\uparrow$, $\psi_\ell^2 = -\mathrm{Re}\,\psi_\ell\downarrow$, $\psi_\ell^3 = \mathrm{Im}\,\psi_\ell^\downarrow$, $\psi_\ell^\alpha \in \mathbb{R}^N$ and E_2 is a two-dimensional unit matrix. Here $\psi_\ell^{\mathbb{H}}$ is a quaternion vector of dimension N.

A linear canonical transformation of the fermions $\{c_n\} \to \{d_\ell\}$, $c_n = U_{n\ell} d_\ell$, which is consistent with the TR invariance, (written in $\{d_\ell\}$) requires that 2×2 matrix $U_{n\ell}$ does commute with the time reversal, that is, $\tilde{J} U_{n\ell}^* J = U_{n\ell} \cong u_{n\ell}^{\mathbb{H}} \in \mathbb{H}$. Supplementing the unitarity of this matrix $U^\dagger U = U U^\dagger = E_{2N}$, $(U)_{n\ell} = U_{n\ell}$, $U \in U(2N, \mathbb{C})$, which guarantees the fermion anticommutation relations of $\{d_{\sigma\ell}\}$'s,

this $2N \times 2N$ matrix U satisfies $\widetilde{U} J_{2N} U = J_{2N},\ J_{2N} = J \otimes E_N,\ (U \in Sp(2N, \mathbb{C}))$. It implies $U \in Sp(N) = U(2N, \mathbb{C}) \cap Sp(2N, \mathbb{C})$ as a $2N$-dimensional matrix. By the standard equivalence, we also have an N-dimensional quaternion matrix $u^{\mathbb{H}} \in M_N(\mathbb{H})$, $(u^{\mathbb{H}})_{n\ell} = u^{\mathbb{H}}_{n\ell} \in \mathbb{H}$. It is constructed from all of the orthonormalized eigen states (KR pairs), $\{\psi^{\mathbb{H}}_\ell\}$, as $u^{\mathbb{H}} = (\psi^{\mathbb{H}}_1, \cdots, \psi^{\mathbb{H}}_N)$, $H\psi_\ell = \epsilon_\ell \psi_] \ell$ $(\epsilon_\ell \neq \epsilon_{\ell'}, \ell \neq \ell')$,

3. Quaternionic structure of many body system with KR degeneracy

The quaternionic structure introduced in the previous Sec.2 is directly extended to the Fock space of the fermion many body states as far as the total number of particles is conserved, since the TR operation Θ does commute with the $Sp(N)$ unitary transformation among the fermion spinors $\{\boldsymbol{c}_n^\dagger\} \to \{\boldsymbol{d}_n^\dagger\}$ and the TR operation Θ, $\boldsymbol{c}_{i\uparrow} \to \boldsymbol{c}_{i\downarrow}$, $\boldsymbol{c}_{i\downarrow} \to -\boldsymbol{c}_{i\uparrow}$ and taking the complex conjugate, has a basis independent meaning. Then it is also applicable for the $S = \frac{1}{2}$ quantum spins by the standard representation $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{c}_i^\dagger \sigma \boldsymbol{c}_i$ (extension to the half-odd-integer spins is trivial by introducing the Hund coupling).

Now let us consider a TR invariant many body hamiltonian $\mathcal{H}$, $[\mathcal{H}, \Theta] = 0$. When the state $|\Psi\rangle$ is an eigen state of the hamiltonian, its time-reversal pair $|\Psi^\Theta\rangle = \Theta|\Psi\rangle$ is also an eigen state. As commented before, we assume the hamiltonian preserves the total fermion number. Then one may discuss an M particle sector separately. The TR operation for this M particle sector is then satisfy $\Theta^2|\psi\rangle = (-)^M|\psi\rangle$.

Now let us further assume that the number of total fermions (1/2 spins) M are odd to have the KR degeneracy. Then we have the following fundamental relation

$$\Theta^2|\psi\rangle = -|\psi\rangle.$$

A generic M particle state is spanned by the Fock basis as

$$|\psi\rangle = \sum \left[\psi_O(i)|O(i)\rangle + \psi_E(i)|E(i)\rangle\right]$$

where $|O(i)\rangle$ and $|E(i)\rangle$ is a basis with odd (even) number of spin up fermions respectively as

$$|O(i)\rangle = c^\dagger_{m_1\uparrow} \cdots c^\dagger_{m_{M_u}\uparrow} c^\dagger_{m_1\downarrow} \cdots c^\dagger_{m_{M_d}\downarrow}|0\rangle\ (M_u : \text{odd},\ M_d : \text{even}))$$

$$|E(i)\rangle = c^\dagger_{m_1\uparrow} \cdots c^\dagger_{m_{M_u}\uparrow} c^\dagger_{m_1\downarrow} \cdots c^\dagger_{m_{M_d}\downarrow}|0\rangle\ (M_u : \text{even},\ M_d : \text{odd}))$$

They are orthonormalized as

$$\langle O(i)|O(j)\rangle = \langle E(i)|E(j)\rangle = \delta_{ij}, \quad \langle O(i)|E(j)\rangle = 0$$

where $i = 1, \cdots, D_F$ is a label of the Fock states. Since the total number of particles is odd, the basis with even up spins $|E(i)\rangle$ is given by that of the odd as

$$|E(i)\rangle = \Theta|O(i)\rangle.$$

Therefore one has (also it is confirmed directly)

$$\Theta|E(i)\rangle = \Theta^2|O(i)\rangle = -|O(i)\rangle$$

As for the generic state $|\psi\rangle$, the TR operation is given as

$$\Theta|\psi\rangle = |\psi^\Theta\rangle = \sum(-\psi^*_E(i)|O(i)\rangle + \psi^*_O(i)|E(i)\rangle)$$

Using this set up, one can directly extend the discussion in the Sec.2. As for the eigen state

$$\psi = \begin{bmatrix} \psi_O \\ \psi_E \end{bmatrix}, \quad \psi_O = \begin{bmatrix} \psi_O(1) \\ \vdots \\ \psi_O(D_F) \end{bmatrix}, \psi_E = \begin{bmatrix} \psi_E(1) \\ \vdots \\ \psi_E(D_F) \end{bmatrix},$$

the KR multiplet of the many body state is given as

$$\Psi = (\psi, \Theta\psi) \equiv \begin{bmatrix} \psi_O & -\psi_E^* \\ \psi_E & \psi_O^* \end{bmatrix} = \psi^0 E + \psi^1 I + \psi^2 J + \psi^3 K$$

where $\psi^0 = \mathrm{Re}\,\psi_O$, $\psi^1 = \mathrm{Im}\,\psi_O$, $-\psi^2 = -\mathrm{Re}\,\psi_E$, $\psi^3 = \mathrm{Im}\,\psi_E$. Orthogonality of the KR pair is also trivial. Similar to the discussion in Sec.2, we identity the KR multiplet as a single state of the quaternion as

$$\Psi \cong \psi^{\mathbb{H}} = \psi^0 + \psi^1 i_{\mathbb{H}} + \psi^2 j_{\mathbb{H}} + \psi^3 k_{\mathbb{H}}$$

Then all of the discussion is trivially transformed into a discussion of the many body states. For example, the quaternionic Berry connection for the many body state is defined as $a^{\mathbb{H}} = (\psi^{\mathbb{H}})^\dagger d\psi^{\mathbb{H}}$. All of the discussion in the paper can be applicable to the many body system. Applications for electronic systems with electron-electron interaction will be given elsewhere.

4. Minimum dimensions for non-trivial Berry connections

To have a non trivial topological structure in the Berry connection, there can be some requirements for the dimension of the parameter space D, which we describe here. Let us first start from a generic consideration of the normalized m-dimensional multiplet $\Psi = (\Psi_1, \cdots, \Psi_m)$, $\Psi^\dagger\Psi = E_m$ and the corresponding m-dimensional non-Abelian Berry connection $A = \Psi^\dagger d\Psi = \Psi^\dagger \partial_\mu \Psi dx^\mu$, which transforms under a gauge transformation $\Psi_g = \Psi g$, $g \in U(m)$, as $A_g = g^{-1}Ag + g^{-1}dg$[8, 42]. The n-th Chern number C_n of this connection is defined as

$$C_n = \left(\frac{i}{2\pi}\right)^n \frac{1}{n!} \int_{M_{2n}} \mathrm{Tr}\, F^n, \quad F = dA + A^2$$

where M_{2n} is an $2n$-dimensional manifold without boundaries $\partial M_{2n} = 0$[43, 44]. Although the field strength F gets modified by the above gauge transformation as $F_g = g^{-1}Fg$, the Chern number is invariant. As for the explicit discussion of the Berry connection, Zumino's generic construction of the topological quantities is quite useful. We shortly summarize a part of them which we require in this article[43, 44]. They read

$$\begin{aligned} \mathrm{Tr}\, F &= d\omega_1(A), \quad \mathrm{Tr}\, F^2 = d\omega_3(A), \\ \omega_1(A) &= \mathrm{Tr}\, A, \qquad \omega_3(A) = \mathrm{Tr}(AdA + \frac{2}{3}A^3) = \mathrm{Tr}(AF - \frac{1}{3}A^3). \end{aligned}$$

The transformation properties are given as

$$\omega_1(A_g) = \omega_1(A) + \mathrm{Tr}(g^{-1}dg), \quad \omega_3(A_g) = \omega_3(A) - \frac{1}{3}\mathrm{Tr}(g^{-1}dg)^3 + d\alpha_2$$

where $\alpha_2 = \mathrm{Tr}(Adgg^{-1})$. Although the Zumino's construction is general for $\mathrm{Tr}\, F^n = d\omega_{2n-1}(A)$, we just need for $n = 1$ and 2, which one can explicitly confirm by a direct calculation.

The Chern number is gauge invariant and it is explicitly given by the gauge invariant projection $P = \Psi\Psi^\dagger$. It is given for the first Chern number[45] but is also done for the higher ones. By taking a differential of P, we have $dP = d\Psi\Psi^\dagger + \Psi d\Psi^\dagger$. Then the following direct calculation below gives a useful formula for gauge invariant quantities as

$$\Psi F \Psi^\dagger = PdP^2P, \quad \mathrm{Tr}\,(PdP^2)^n = \mathrm{Tr}\, F^n$$

It obeys from the following observation

$$\begin{aligned}
(dP)^2 &= d\Psi\Psi^\dagger d\Psi\Psi^\dagger + \Psi d\Psi^\dagger d\Psi\Psi^\dagger + d\Psi\Psi^\dagger\Psi d\Psi^\dagger + \Psi d\Psi^\dagger\Psi d\Psi^\dagger \\
&= -d\Psi d\Psi^\dagger\Psi\Psi^\dagger + \Psi d\Psi^\dagger d\Psi\Psi^\dagger + d\Psi d\Psi^\dagger - \Psi\Psi^\dagger d\Psi d\Psi^\dagger \\
&= -d\Psi d\Psi^\dagger P + \Psi d\Psi^\dagger d\Psi\Psi^\dagger + d\Psi d\Psi^\dagger - Pd\Psi d\Psi^\dagger \\
P(dP)^2P &= -Pd\Psi d\Psi^\dagger P + P\Psi d\Psi^\dagger d\Psi\Psi^\dagger P + Pd\Psi d\Psi^\dagger P - Pd\Psi d\Psi^\dagger P \\
&= -Pd\Psi d\Psi^\dagger P + P\Psi d\Psi^\dagger d\Psi\Psi^\dagger P \\
&= -\Psi\Psi^\dagger d\Psi d\Psi^\dagger\Psi\Psi^\dagger + \Psi\Psi^\dagger\Psi d\Psi^\dagger d\Psi\Psi^\dagger\Psi\Psi^\dagger \\
&= \Psi\Psi^\dagger d\Psi\Psi^\dagger d\Psi\Psi^\dagger + \Psi d\Psi^\dagger d\Psi\Psi^\dagger \\
&= \Psi\big[d\Psi^\dagger d\Psi + (\Psi^\dagger d\Psi)^2\big]\Psi^\dagger = \Psi F\Psi^\dagger
\end{aligned}$$

where the normalization $\Psi^\dagger\Psi = E_M$ implies $\Psi^\dagger d\Psi = -d\Psi^\dagger\Psi$, $P^2 = P$ and $dA = d\Psi^\dagger d\Psi$. Then the Chern number is written as an explicit gauge invariant form as

$$C_n = (\frac{i}{2\pi})^n\frac{1}{n!}\int_{M_{2n}}\mathrm{Tr}\,\big[P(dP)^2P\big]^n = (\frac{i}{2\pi})^n\frac{1}{n!}\int_{M_{2n}}\mathrm{Tr}\,\big[P(dP)^2\big]^n.$$

As for the TR invariant system with the KR degeneracy, we identify the multiplet of the dimension $2M$ to the quaternionic one with the dimension M as $\Psi = (\Psi_1,\cdots,\Psi_M) \cong \psi^{\mathbb{H}}$. Then a gauge transformation $\psi^{\mathbb{H}}_g = \psi^{\mathbb{H}}g$, $g \in Sp(M)$ preserves the TR invariant linear space spanned by $\psi^{\mathbb{H}}$. Now the quaternionic Berry connection $a^{\mathbb{H}} = (\psi^{\mathbb{H}})^\dagger d\psi^{\mathbb{H}}$ and corresponding field strength $f^{\mathbb{H}} = da^{\mathbb{H}} + (a^{\mathbb{H}})^2$ are defined as usual. Their transformation properties are also standard as $a^{\mathbb{H}}_g = (\psi^{\mathbb{H}}_g)^\dagger d\psi^{\mathbb{H}}_g = g^{-1}a^{\mathbb{H}}g + g^{-1}dg$ and $f^{\mathbb{H}}_g = da^{\mathbb{H}}_g + (a^{\mathbb{H}}_g)^2 = g^{-1}f^{\mathbb{H}}g$. The n-th Chern number with *even* n, C_n is defined as (Since the C_n is intrinsically integer, it suggests vanishing C_n for odd n)

$$C_n = \left(\frac{-1}{4\pi^2}\right)^{n/2}\frac{1}{n!}\int_{M_n}\mathrm{Tr}_M\,T\,(f^{\mathbb{H}})^n = \left(\frac{-1}{4\pi^2}\right)^{n/2}\frac{1}{n!}\int_{M_n}\mathrm{Tr}_M\,T\,[p^{\mathbb{H}}(dp^{\mathbb{H}})^2]^{n/2}$$

where $Tx^{\mathbb{H}} = x + \bar{x} = 2x^0 \in \mathbb{R}$ for a quaternion $x = x^0 + x^1 i_{\mathbb{H}} + x^2 j_{\mathbb{H}} + x^3 k_{\mathbb{H}}$ and the quateronic projection is $p^{\mathbb{H}} = \psi^{\mathbb{H}}(\psi^{\mathbb{H}})^\dagger$. In the following, we omit the symbol $^{\mathbb{H}}$ and simply use the lower character for the quaternionic notation if the situation is clear.

Since the multiplet and the Berry connection have a gauge freedom, one needs to fix it for the connection to be well-defined. As for the generic multiplet without the KR degeneracy, the gauge is specified by an arbitrary but given multiplet Φ as $\Psi_\Phi = P\Phi N_\Phi^{-1/2}$ where P is a gauge independent projection and the normalization matrix $N_\Phi = \Phi^\dagger P\Phi$ which is also gauge invariant and is semi-positive definite[11]. When one can use this single gauge over the whole parameter space, the Berry connection is trivial. Generically, however, the normalization matrix may have zero eigen values as $\det N_\Phi(^\exists x_\Phi) = 0$. Then near this zero, x_Φ, this gauge is singular since one can not normalize. One needs to use the other gauge, say, $\psi_{\Phi'}$ by taking Φ'. Since $\det N_{\Phi'}(x_\Phi) \neq 0$, generically, one can express the projection by the multiplet explicitly as $P = \Psi_{\psi'}\Psi_{\psi'}^\dagger$ and the normalization matrix is factorized as $N_\Phi = \Phi^\dagger P\Phi = \eta^\dagger_{\Phi'\Phi}\eta_{\Phi'\Phi}$, $\eta_{\Phi'\Phi} \equiv \Psi^\dagger_{\Phi'}\Phi$. One may write it as $\eta_\Phi = \Psi^\dagger\Phi$ when one does not need to specify the gauge. Now it is clear that the singularity is specified by

$$\det\eta_{\Phi'\Phi} = 0 \rightleftarrows \mathrm{Re}\,\big(\det\eta_{\Phi'\Phi}\big) = \mathrm{Im}\,\big(\det\eta_{\Phi'\Phi}\big) = 0$$

since this determinant is complex, $\det\eta_\Phi(x) \in \mathbb{C}$. Generically one does not have zeros when the dimension of the parameter space is too low and the Berry connection is

trivial. To have a non trivial topological structure the dimension of the parameter space has to satisfies $D \geq D_{min} = 2$, since the condition to have the singularities is given by the two real equations. A two-dimensional magnetic Brilluine zone to discuss the Hall conductance as the first Chern number is this minimiun space where the singularities occur in points[6]. Note that the gauge transformation between the two gauges by Φ and Φ', $\Psi_{\Phi'} = \Psi_\Phi g_{\Phi\Phi'}$, is explicitly given by

$$\begin{aligned}\Psi_\Phi &= \Psi_{\Phi'}\Psi_{\Phi'}^\dagger \Phi N_\Phi^{-1/2} = \Psi_{\Phi'} g_{\Phi'\Phi},\\ g_{\Phi'\Phi} &= \Psi_{\Phi'}^\dagger \Phi N_\Phi^{-1/2} = (N_{\Phi'})^{-1/2}\Phi'^\dagger P \Phi (N_\Phi)^{-1/2} \in U(M).\end{aligned}$$

The unitarity is confirmed as

$$\begin{aligned}g_{\Phi'\Phi} g_{\Phi'\Phi}^\dagger &= (N_{\Phi'})^{-1/2}\Phi'^\dagger P\Phi(N_\Phi)^{-1}\Phi^\dagger P\Phi'(N_{\Phi'})^{-1/2}\\ &= (N_{\Phi'})^{-1/2}\eta_{\Phi'}^\dagger \eta_\Phi (N_\Phi)^{-1}\eta_\Phi^\dagger \eta_{\Phi'}(N_{\Phi'})^{-1/2} = (N_{\Phi'})^{-1/2}\eta_{\Phi'}^\dagger \eta_{\Phi'}(N_{\Phi'})^{-1/2} = E_M\end{aligned}$$

and $g_{\Phi'\Phi}^\dagger g_{\Phi'\Phi} = E_M$ similarly.

As for a systems with the KR pairs, let us here consider the simpest $M = 1$ case. Now starting from the gauge invariant projection p into the degenerate KR space, the gauge is fixed by an aribitrary quaternion vector $\phi \in \mathbb{H}^N$ as

$$\psi_\phi = p\phi N_\phi^{-1/2}, \quad N_\phi = \phi^\dagger p \phi = N(\eta_\phi) \in \mathbb{R}, \quad \eta_\phi = \psi^\dagger \phi \in \mathbb{H}$$

where $N(x) = \bar{x}x = (x^0)^2 + (x^1)^2 + (x^2)^2 + (x^3)^2$ is a norm of a quaternion $x \in \mathbb{H}$. This gauge is again well defined only if $N_\phi \neq 0$. Note that although η_ϕ itself is gauge dependent but the norm $N(\eta_\phi)$ is gauge invariant as $N(\psi_g^\dagger \phi) = N(\bar{g}\psi^\dagger \phi) = N(g)N(\psi^\dagger\phi) = N(\psi^\dagger \phi)$, ($\psi_g = \psi g$, $g \in Sp(1)$). Therefore we do not need to specify the gauge for $N(\eta_\phi)$.

Near the singular point of this gauge, one needs to use the other gauge by ϕ'. Then the condition of the vanishing norm $N_\phi = N(\eta_{\phi'\phi})$, is expressed as

$$\eta_{\phi'\phi} = 0 \rightleftarrows T\big(\eta_{\phi'\phi}\big) = T\big(i_{\mathbb{H}}\eta_{\phi'\phi}\big) = T\big(j_{\mathbb{H}}\eta_{\phi'\phi}\big) = T\big(k_{\mathbb{H}}\eta_{\phi'\phi}\big) = 0.$$

It clearly shows that the singularity may occur in the parameter space of the dimension $D \geq D_{min}^{\mathrm{KR}} = 4$. The gauge transformation is also give as

$$\psi_\phi = \psi_{\phi'} g_{\phi'\phi}, \quad g_{\phi'\phi} = [N(\phi')]^{-1/2}(\phi')^\dagger p \phi [N(\phi)]^{-1/2} \in Sp(1).$$

When the dimension of the parameter space is less than this minimum dimension, one can generically take a single patch over the whole parameter space. Since the base space to define the Chern numbers are assumed to be without boundaries, it implies that the Chern number is vanishing for $\dim M_{2n} = 2n < D_{min}^{\mathrm{KR}} = 4$. Then the natural quantities to have non trivial topological structure by the Chern numbers are C_1 for the generic case and C_2 for the system with the KR degeneracy.

Also note that the normalization of the KR pair in quaternion notation $\psi^\dagger\psi = 1$ gives $0 = \psi^\dagger d\psi + d\psi^\dagger \psi = \psi^\dagger d\psi + \widetilde{d\psi^\dagger \psi} = \psi^\dagger d\psi + \widetilde{\psi} d\bar{\psi} = T(\psi^\dagger d\psi) = T(a)$, which implies the first Chern number is vanishing that is consistent with the generic argument [29, 46]. Then let us focus on the 2nd Chern number with the KR degeneracy.

5. Degeneracies to Monopoles with/without KR degeneracy

As was pointed out by Berry, the generic degeneracy of a complex hamiltonian has a co-dimension $d_C = 3$[8], that is, the minimum hamiltonian ($N = 2$) to describe the degeneracy (at $E = \mathrm{Tr}\, H_{\mathbb{C}} = 0$) is a complex hermite 2×2 matrix

$H_{\mathbb{C}}$ which is expanded by the Pauli matrix with 3 dimensional real coefficients $\boldsymbol{R}(x) = (R_1(x), R_2(x), R_3(x)) \in \mathbb{R}^3$ as

$$H_{\mathbb{C}}(x) = \begin{bmatrix} R_3 & z \\ \bar{z} & -R_3 \end{bmatrix}, \quad z = R_1 - iR_2$$

where $R_3 = R_3(x) \in \mathbb{R}$, $z = z(x) \in \mathbb{C}$. Similarly the system with the KR degeneracy does have a co-dimension $d_H = 5$ as pointed out by Avron et al.[29, 46]. Then the minimum model ($N = 2$, $E = \mathrm{Tr}\, H_{\mathbb{H}} = 0$) is realized by the following quaternionic hermite hamiltonian

$$H_{\mathbb{H}}(x) = \begin{bmatrix} Q_5 & q \\ \bar{q} & -Q_5 \end{bmatrix}, \quad q = q_0 + q_1 i_{\mathbb{H}} + q_2 j_{\mathbb{H}} + q_3 k_{\mathbb{H}}$$

where $Q_5 = Q_5(x) \in \mathbb{R}$, $q_i(x) \in \mathbb{R}$, $(i = 1, 2, 3)$ and $q = q(x) \in \mathbb{H}$. These $\boldsymbol{Q} = (Q_1, Q_2, Q_3, Q_4, Q_5) \in \mathbb{R}^5$, $(Q_1 = q_1, Q_2 = q_2, Q_3 = q_3, Q_4 = q_0)$ form 5 dimensional parameters of the minimum model with the KR degeneracy.

The above observation suggests strong analogy between the systems with and without the KR degeneracy, which we pursuit in this paper. There is also a topological correspondence as discussed below (See Fig.1). Actually it is more than analogy and there exists a mapping by $R_3 \to Q_5$ and $z(\in \mathbb{C}) \to q(\in \mathbb{H})$ as one can see. The origins of the parameter spaces $\boldsymbol{R} = 0$ and $\boldsymbol{Q} = 0$ give degeneracies which bring singularities for the each Berry connections. They are the Dirac monopole[1] and the Yang monopole[47, 48, 49, 30, 31, 27, 32]. The Yang monopole is literally a quaternionic Dirac monopole up to its topological structure.

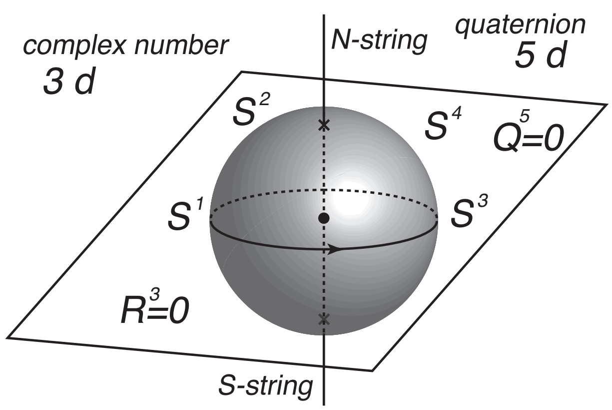

Figure 1. Topological objects and singularities for the Dirac monopole and the Yang monopole.

5.1. Dirac monopole and the first Chern number

Due to a simple observation, $H_{\mathbb{C}}^2 = R^2 E_2$, $R = |\boldsymbol{R}|$, the energies of $H_{\mathbb{C}}$ are $\pm R = \sqrt{|z|^2 + R_3^2}$. Then the degeneracy occurs at the origin in the 3 dimensional $\boldsymbol{R}$ space $\mathbb{R}^3$. Away from this degeneracy, the eigen state of the energy $\pm R$ subspace is well defined by the projection $P_{\pm} = \frac{1}{2}(1 \pm H_{\mathbb{C}}/R)$. As for the base manifold to define the first Chern number, for simplicity, let us take the 2-sphere $S^2 = \{\boldsymbol{R} | R = 1\} \subset \mathbb{R}^3$ as for M_{2n}, $n = 1$ (Fig.1). Then the possible singularities of the Berry connection

can be points on the S^2 by the generic consideration before. When one considers a generic base space in $\mathbb{R}^3$, these singularities form lines, which correspond to the Dirac strings[50]. The gauge invariant projection into each eigen subspace is explicitly given as $P_\pm = \frac{1}{2}\begin{bmatrix} 1 \pm R_3 & \pm z \\ \pm\bar{z} & 1 \mp R_3 \end{bmatrix}$. In the following, let us consider a positive energy subspace $P = P_+$. Taking a gauge by $\Phi_N = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, the normalized state on S^2, $(|z|^2 + R_3^2 = 1)$, is given as a $\Psi_N = P\Phi_N N_N^{-1/2}$ with $N_N = \Phi_N^\dagger P \Phi_N = \frac{1}{2}(1 + R_3)$. Since this gauge is only singular at the south pole $R_3 = -1$, we can safely use $\Psi_N = \frac{1}{\sqrt{2}}\begin{bmatrix} (1 + R_3)^{+1/2} \\ \bar{z}(1 + R_3)^{-1/2} \end{bmatrix}$ for the north hemisphere S_N^2 ($R_3 \geq 0$). As for the south hemisphere, we needs to use the other gauge, say, by $\Phi_S = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Then the normalized state is given similarly as $\Psi_S = P_{\mathbb{C}}\Phi_S N_S^{-1/2} = \frac{1}{\sqrt{2}}\begin{bmatrix} z(1 - R_3)^{-1/2} \\ (1 - R_3)^{+1/2} \end{bmatrix}$, $N_S = \Phi_S^\dagger P_{\mathbb{C}} \Phi_S = \frac{1}{2}(1 - R_3)$, which is regular everywhere on the south hemisphere S_S^2 ($R_3 \leq 0$).

The gauge transformation, $g_{SN}^{\mathbb{C}}$, between them, $\Psi_N = \Psi_S g_{SN}^{\mathbb{C}}$, is given by the generic formula before as

$$g_{SN}^{\mathbb{C}} = N_S^{-1/2}\Phi_S^\dagger P_{\mathbb{C}} \Phi_N N_N^{-1/2} = \bar{z}/|z|.$$

This is regular except the north and south poles $R_3 = \pm 1$.

The first Chern number of the Berry connection is easily evaluated using these two gauges and the gauge transformation, $A_N = g_{SN}^{-1} A_S g_{SN} + g_{SN}^{-1} dg_{SN}$

$$\begin{aligned}
C_1 &= \frac{i}{2\pi}\int_{S^2} \mathrm{Tr}\, F = \frac{i}{2\pi}\int_{S^2} d\omega_1(A) = \frac{i}{2\pi}\bigg(\int_{S_N^2} d\omega_1(A_N) + \int_{S_S^2} d\omega_1(A_S)\bigg) \\
&= \frac{i}{2\pi}\bigg(\int_{\partial S_N^2} \omega_1(A_N) + \int_{\partial S_S^2} \omega_1(A_S)\bigg) = \frac{i}{2\pi}\int_{S^1 = \partial S_N^2} \big(\omega_1(A_N) - \omega_1(A_S)\big) \\
&= W_{S^1}(g_{SN}^{\mathbb{C}})
\end{aligned}$$

where $S^1 = \partial S_N^2 = \partial S_S^2$ is an equator $S^1 = \{\boldsymbol{R} | R = 1, R_3 = 0\}$ and $W_{S^1}(g_{SN}^{\mathbb{C}})$ is a winding number of the map from the 1-sphere (circle) $S^1 = \{(R_1, R_2) | R_1^2 + R_2^2 = 1\}$ to $U(1) \cong S^1 = \{z \big| |z|^2 = 1\} \in \mathbb{C}$ as

$$W_{S^1}(g_{SN}^{\mathbb{C}}) = \frac{i}{2\pi}\int_{S^1} (g_{SN}^{\mathbb{C}})^{-1} dg_{SN}^{\mathbb{C}} = -1.$$

This winding number can be evaluated by several ways. Since this is invariant against a rotation in S^1 ($g \to e^{i\theta} g$), we write it in a local coordinate near $R_1 = 0$ and $R_2 = 1$ as $g = -i$, $dg = dR_1$ as $W_{S^1}(g_{SN}^{\mathbb{C}}) = (i/2\pi)\int_{S^1} dR_1/(-i) = -\int_{S^1} dR_1/(2\pi) = -1$ where $\int_{S^1} dR_1 = 2\pi$ is a volume (length) of the circle S^1. Also using the explicit form $g_{SN}^{\mathbb{C}} = e^{i\mathrm{Arg}\,(R_1 + iR_2)}$, we have $\int_{S^1} g^{-1} dg = i\int_{S^1} d\,\mathrm{Arg}\,(R_1 + iR_2) = 2\pi i$.

Considering the S^2 as a boundary of the solid sphere V_3 ($\partial V_3 = S^2$), naive application of the Stokes (Gauss) theorem, $C_1 = \displaystyle\int_{V_3} dF$, suggests $\frac{i}{2\pi} dF = -\delta^{(3)}(\boldsymbol{R})$ since $dF = d^2 A = 0$ as far as the Berry connection is well-defined except the origin. This is the *Dirac monopole* at the origin of the 3-dimensional $\boldsymbol{R}$ space where the degeneracy of the generic complex hamiltonian occurs[1].

5.2. Yang monopole as a quateronic Dirac monopole

The discussion with the KR degeneracy can be done quite analogously. Let us again start from a simple observation $H_{\mathbb{H}}^2 = Q^2 E_5$, $Q = |\boldsymbol{Q}|$, which implies that eigen energies of the KR multiplets are $\pm Q = \pm\sqrt{|q|^2+Q_5^2}$, $|q| = \sqrt{N(q)} \in \mathbb{R}$, and the additional degeneracy to the Kramers degeneracy occurs at the origin in the 5-dimensional $\boldsymbol{Q}$ space $\mathbb{R}^5$ (Fig.1). A projection into the positive energy KR multiplet is defined as $p = \frac{1}{2}(1 + H_{\mathbb{H}}/Q)$. Similar to the discussion above, let us take a 4-sphere $S^4 = \{\boldsymbol{Q}\big|Q = 1\} \subset \mathbb{R}^5$ as the base space M_{2n}, $(n = 2)$ to define the second Chern number C_2. Then the generic singularities of the KR multiplet are again points on S^4, which make lines in the $\mathbb{R}^5$ when one considers a generic 4 dimensional surface as a base space ("Yang" strings). To be more specific, let us take a gauge by taking a quaternion vector with 2 components $\phi_N = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathbb{H}^2$. Then the normalized KR multiplet is given, in the north pole gauge (regular in the north hemisphere $S_N^4(Q_5 \geq 0)$), as

$$\psi_N = p\phi_N N_N^{-1/2} = \frac{1}{\sqrt{2}} \begin{bmatrix} (1+Q_5)^{+1/2} \\ \bar{q}(1+Q_5)^{-1/2} \end{bmatrix}$$

where $N_N = \phi_N^\dagger p \phi_N = \frac{1}{2}(1+Q_5)$. This gauge is only singular at the south pole $Q_5 = -1$ on the S^4. The other gauge by $\phi_S = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ also defines the multiplet (in the south pole gauge)

$$\psi_S = p\phi_S N_S^{-1/2} = \tfrac{1}{\sqrt{2}} \begin{bmatrix} q(1-Q_5)^{-1/2} \\ (1-Q_5)^{+1/2} \end{bmatrix}$$

where $N_S = \phi_S^\dagger p \phi_S = \frac{1}{2}(1-Q_5)$. This is regular in the south hemisphere $S_S^4(Q_5 \leq 0)$. The gauge transformation between them is also calculated as

$$\psi_S^{\mathbb{H}} = g_{SN}^{\mathbb{H}} \psi_N^{\mathbb{H}}, \quad g_{SN}^{\mathbb{H}} = \bar{q}/|q| \in Sp(1) = \{g \in \mathbb{H}|N(g) = 1\}$$

Now let us calculate the second Chern number in the quaternionic notation as

$$\begin{aligned} C_2 &= -\frac{1}{8\pi^2}\int_{S^4} Tf^2 = -\frac{1}{8\pi^2}\int_{S^4} d\omega_3(a) = -\frac{1}{8\pi^2}\left(\int_{S_N^4} d\omega_3(a_N) + \int_{S_S^4} d\omega_3(a_S)\right) \\ &= -\frac{1}{8\pi^2}\int_{S^3}\big(\omega_3(a_N) - \omega_3(a_S)\big) = \frac{1}{24\pi^2}\int_{S^3} T((g_{SN}^{\mathbb{H}})^{-1} dg_{SN}^{\mathbb{H}})^3 \\ &\equiv W_{S^3}(g_{SN}^{\mathbb{H}}) = -1 \end{aligned}$$

where $S^3 = S^4\big|_{Q_5=0} = \{(q_1,q_2,q_3,q_0)\big||q| = 1\}$ is an equator, $\omega_3(a) = T(ada + \frac{2}{3}a^3)$ and $W_{S^3}(g_{SN}^{\mathbb{H}})$ is the Pontrjagin number of the map $S^3 \to Sp(1) \cong S^3$ that is a covering degree, which is intrinsically integer. Here we used $\int_{S^3} d\alpha_2 = \int_{\partial S^3} \alpha_2 = 0$ since the gauge is regular on the S^3 which does not have boundaries. This Pontrjagin number is explicitly evaluated[51]. Since it is invariant for the change $q \to q\xi$, $|\xi| = 1$ that induces a rotation of S^3, it is enough to evaluate it near $q = 1$ ($q_0 = 1, q_1 = q_2 = q_3 = 0$), where $T(q^{-1}dq)^3 = 3!T(i_{\mathbb{H}}j_{\mathbb{H}}k_{\mathbb{H}})dq_1dq_2dq_3 = -12dq_1dq_2dq_3$. Then we have $C_2(\boldsymbol{Q}) = W_{S^3}(g_{SN}^{\mathbb{H}}) = \frac{1}{24\pi^2}(-12\cdot 2\pi^2) = -1$ where $2\pi^2$ is a volume of the S^3.

Again writing the S^4 as a surface of a 5 dimensional solid sphere $V_5 = \{\boldsymbol{Q}\big||\boldsymbol{Q}| \leq 1\}$, $\partial V_5 = S^4$, one may write symbolically $dT(f^2) = -\delta^{(5)}(\boldsymbol{Q})$ by a simple application of the Stokes theorem $\int_{V_5} dT(f^2) = \int_{\partial V_5} T(f^2) = -1$, since $dT(f^2) = d^2\omega_3 = 0$ away from the origin where the singularity exists. The origin of the 5-dimensional $\boldsymbol{Q}$ space,

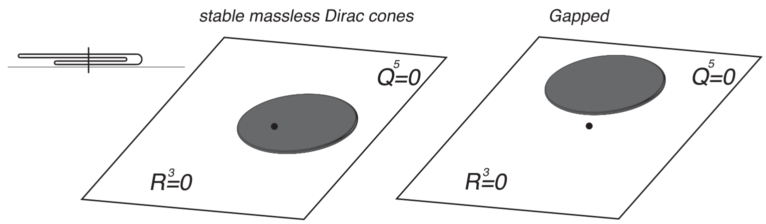

Figure 2. Collapsed images of the maps into the hyperplanes $M_2 \to \boldsymbol{R} \subset \mathbb{R}^2$: $(R_3 = 0)$ and $M_4 \to \boldsymbol{Q} \subset \mathbb{R}^4$: $(R_3 = 0)$ with the chiral symmetric minimum models.

$\boldsymbol{Q} = 0$, is a singular point for the Berry connection due to the additional degeneracy (4-fold) and it induces the Yang's monopole in 5-dimensions[47] which locates at $\boldsymbol{Q} = 0$ (the charge is -1). This explicit demonstrates that *the Yang monopole is a quaternioninc Dirac monopole.*

5.3. *Chiral symmetry and topological stability of the Dirac cones*

For simplicity, we have assumed the 2-sphere and the 4-sphere as the parameter spaces M_2 and M_4. In a generic situation, let us consider the Chern numbers of the models $H_{\mathbb{C}}(\boldsymbol{R}(x))$, $(x \in M_2)$ and $H_{\mathbb{H}}(\boldsymbol{Q}(x))$ $(x \in M_4)$. Assuming the energy gaps never collapses, the images $\boldsymbol{R}(M_2) \subset \mathbb{R}^3$ and $\boldsymbol{Q}(M_4) \subset \mathbb{R}^5$ are deformed into the spheres S^2 and S^4 without changing the Chern numbers. This is the topological stability and these topological numbers are given by the covering degrees of the maps as[52]

$$C_1 = -\deg \boldsymbol{R}(M_2) : M_2 \to S^2, \quad C_2 = -\deg \boldsymbol{Q}(M_4) : M_4 \to S^4.$$

To have the well-defined Chern numbers, the gap has to be open always. However in some situation, the gap may collapse. Generically speaking, this is accidental (accidental degeneracy). In other words, one may need to fine tune physical parameters which occurs at a quantum critical point. By imposing some restriction by symmetry, the situation may change and the gap closing has a topological stability. Let us here impose a "chiral symmetry" and restrict the parameter space. The chiral operator in the minimum model is given by $\Gamma = \sigma_3$, $\Gamma^2 = 1$. The hamiltonians of the minimum models satisfy $\{H_{\mathbb{C}}, \Gamma\} = 2R_3$, $\{H_{\mathbb{H}}, \Gamma\} = 2Q_5$. That is, the equators (S^1 and S^3 respectively) are characterized as the chiral symmetrical spaces

$$\{H_{\mathbb{C}}(\boldsymbol{R}), \Gamma\} = 0 \ (\boldsymbol{R} \in S^1), \quad \{H_{\mathbb{H}}(\boldsymbol{Q}), \Gamma\} = 0 \ (\boldsymbol{Q} \in S^3)$$

When the hamiltonians do have the chiral symmetry, the parameter spaces $\boldsymbol{R}(M_2$ (for $H_{\mathbb{C}}$) and $\boldsymbol{Q}(M_4)$ (for $H_{\mathbb{H}}$) are collapsed into the hyperplane $\mathbb{R}^2(R_3 = 0)$ and $\mathbb{R}^3(Q_5 = 0)$. Then we have two situations for the images $\boldsymbol{R}(M_2)/\boldsymbol{Q}(M_4)$ (See Fig.2). The one case is that the $\boldsymbol{R}(M_2)/\boldsymbol{Q}(M_4)$ includes the origin and in the other case, it does not. When the image includes the origin, it implies the energy gap collapses and is the gap is linearly vanishing as a function of the parameter x generically. It brings a Dirac-cone like energy dispersion. The doubling is also topologically clear (See the inset of the Fig.2). This Dirac cones are generically topologically stable, that is, stable against for small but finite perturbation since the images $\boldsymbol{R}(M_2) \subset \mathbb{R}^2$ and $\boldsymbol{Q}(M_4) \subset \mathbb{R}^4$. These topological stability of the Dirac cones in 2/4 dimensions are discussed in relation to the graphene and Nielsen-Ninomiya theorem [53, 54, 55].

6. Symmetry protected $\mathbb{Z}_2$ quantization

As discussed, the Chern numbers are gauge invariant and intrinsically integer which apparently have a topological stability. It implies that the quantization is stable for small but finite perturbation for the hamiltonian. This topological stability does play a crucial role, for example, in the theory of the quantized Hall effects. Note that the dimension of the parameter space to define the Chern numbers is necessarily even. The winding number W_{S^1} and the Pontrjagin index W_{S^3} are also topological as their definitions and defined for the spaces with odd dimensions. Further in odd dimensions, one may also define quantized quantities if one imposes additional symmetry requirements. They are generalizations of the Berry phase and are generically gauge dependent as a phase of the wave function[8, 13]. It implies these quantities are essentially quantum mechanical and do not have any classical correspondents. They also have a fundamental advantage in the identification of the topological ordered states[12, 13]. An example is a $\mathbb{Z}_2$-quantization of the Berry phase for the TR invariant system without the KR degeneracy $\Theta^2 = 1$ [13, 15, 14, 16]. The focus of this section is to extend the idea and supplies a generic condition for the $\mathbb{Z}_2$-quantization.

Now let us start by defining generic Berry phases $\gamma_1(A)$ and $\gamma_3(a)$ as

$$\gamma_1(A) = \frac{i}{2\pi}\int_{S^1}\omega_1(A), \quad \gamma_3(a) = -\frac{1}{8\pi^2}\int_{S^3}\omega_3(a)$$

where $\gamma_1(A)$ is for a generic system (without degeneracy $M = 1$) and $\gamma_3(a)$ is for a system with the KR degeneracy using a quaternionic notation before. Note here that the same topological quantity by the integral of the Chern-Simons form is discussed in several papers[56, 28, 37]. They are not invariant for the gauge transformation $A_g = g^{-1}Ag + g^{-1}dg$ ($g \in U(1)$) and $a_g = g^{-1}ag + g^{-1}dg$ ($g \in Sp(1)$). Therefore they are not well defined (as they are) but are gauge independent and well-defined in modulo 1 as[13]

$$\gamma_1(A_g) = \gamma_1(A) + W_{S^1}(g) \equiv \gamma_1(A), \quad \gamma_3(a_g) = \gamma_3(a) + W_{S^3}(g) \equiv \gamma_3(a)$$

since the gauge dependence is due to a non trivial large gauge transformation. These contribution are topological and integers as $W_{S^1}(g) \in \mathbb{Z}$ and $W_{S^1}(g) \in \mathbb{Z}$[13] as far as the gauge transformations are regular over the S^1 and S^3. A phase factor of the Berry phase $e^{i2\gamma}$ ($\gamma = 2\pi\gamma_1$) is gauge independent and is a well defined quantity (observed as a geometrical phase) but the phase γ itself is gauge dependent[8, 13].

Generically speaking, these generic Berry phases γ_1 and γ_3 may take any real values even in modulo 1. However they can be quantized when the system obey some symmetry requirement which we discuss below.

6.1. $\mathbb{Z}_2$ quantization of TR invariant system without KR degeneracy

Let us first consider a TR invariant system without the KR degeneracy[13, 14, 15, 16]. This is realized for quantum systems with even number of quantum spins. Since the hamiltonian $\mathcal{H}$ does commute with the TR operator Θ, which is anti-unitary, $[\mathcal{H}, \Theta] = 0$

$$\mathcal{H}(x)\psi(x) = \epsilon(x)\psi(x), \quad \mathcal{H}(x)\psi^\Theta(x) = \epsilon(x)\psi^\Theta(x), \quad \psi^\Theta \equiv \Theta\psi$$

Due to the uniqueness of the state, ψ and ψ^Θ are only different in phase, that is, the corresponding Berry connections $A = \psi^\dagger d\psi$ and $A^\Theta = (\psi^\Theta)^\dagger d\psi^\Theta$ are transformed each

other by some gauge transformation g, $A = g^{-1}A^{\theta}g + g^{-1}dg$, as $\gamma_1(A) \equiv \gamma_1(A^{\Theta}) \bmod 1$, since the gauge transformation is, generically, well defined on the parameter space $x \in S^1$. Also the time reversal operation for the many spin state ψ is written as $\Theta = U\mathcal{K}$ with some parameter independent unitary transformation U. Then the Berry connection is written as

$$A^{\Theta} = (\psi^{\Theta})^{\dagger} d\psi^{\Theta} = \mathcal{K}A = -A$$

since the normalization $\psi^{\dagger}\psi = 1$ implies that $0 = (d\psi^{\dagger})\psi + \psi^{\dagger}d\psi = \widetilde{d\psi^{\dagger}\psi} + A = \widetilde{\psi}d\psi^{*} + A = A^{*} + A$. Now we have two conditions for the Berry phases

$$\gamma_1(A) \equiv \gamma_1(A^{\Theta}) = -\gamma_1(A) \quad \bmod 1$$

Therefore allowed values of the Berry phase are restricted into two as $\gamma_1(A) = 0, \frac{1}{2}$. This is the $\mathbb{Z}_2$-quantization of the Berry phase for the unique TR invariant state.

In most of the application[13, 14, 15, 16], we have used a $U(1)$ twist $e^{i\theta}$, $\theta : 0 \to 2\pi$ as a parameter. In this case, the condition of the $\mathbb{Z}_2$-quantization is reformulated from a more generic point of view (See below).

6.2. $\mathbb{Z}_2$-quantization by inversion/reflection equivalence

Similar quantizations protected by symmetry occur for the generic Berry phases, γ_1 and γ_3, when the system (with parameter) does satisfy the following *inversion/reflection equivalence*. The inversion/reflection equivalence implies that existence of the unitary operator $U_{\mathcal{I}}$ or $U_{\mathcal{R}}$

$$H(x_{\mathcal{I}}) = U_{\mathcal{I}}^{\dagger}H(x)U_{\mathcal{I}}, \quad \text{or} \quad H(x_{\mathcal{R}}) = U_{\mathcal{R}}^{\dagger}H(x)U_{\mathcal{R}}$$

where $H(x)$ is a complex or a quaternionic hamiltonian for $x \in S^1$ or $x \in S^3$ respectively. The inversion in the parameter space is defined as $x_{\mathcal{I}} = -x$ and the reflection is one of the following three, $x_{\mathcal{R}} = (-x_1, x_2, x_3)$, $x_{\mathcal{R}} = (x_1, -x_2, x_3)$, and $x_{\mathcal{R}} = (x_1, x_2, -x_3)$. As for the $x \in S^1$ case, the reflection is the same as the inversion. This is a *sufficient* condition for the $\mathbb{Z}_2$-quantization.

Although we use the quaternion notation with the reflection below (with the KR degeneracy), it is also true for the inversion and the complex cases. The isolated KR multiplet, denoted as $\psi(x)$ with the energy $E(x)$, satisfies $H(x_{\mathcal{R}})\psi(x_{\mathcal{R}}) = U_{\mathcal{R}}^{\dagger}H(x)U_{\mathcal{R}}\psi(x_{\mathcal{R}}) = E(x_{\mathcal{R}})\psi(x_{\mathcal{R}})$ due to the reflection equivalence. It implies

$$H(x)\psi_{\mathcal{R}}(x) = E(x_{\mathcal{R}})\psi_{\mathcal{R}}(x)$$

where $\psi_{\mathcal{R}}(x) = U_{\mathcal{R}}\psi(x_{\mathcal{R}})$. Since the unitary equivalence between $H(x)$ and $H(x_{\mathcal{R}})$ implies that all of the eigen values are equal with each other, we may generically assume $E(x_{\mathcal{R}}) = E(x)$ supplementing a unitary transformation of reshuffling the KR degenerated eigen spaces. Now, as for the isolated eigen space of the KR multiplet, $\psi(x)$ and $\psi_{\mathcal{R}}(x)$ are different just in $Sp(1)$ phase, which implies that the corresponding Berry connections are gauge equivalent, $\psi_{\mathcal{R}}(x) = \psi(x)g$, $^{\exists}g \in Sp(1)$,

$$a_{\mathcal{R}}(x) = \psi_{\mathcal{R}}^{\dagger}(x)d\psi_{\mathcal{R}}(x) = \psi^{\dagger}(x_{\mathcal{R}})d\psi(x_{\mathcal{R}}) = a(x_{\mathcal{R}}) = g^{-1}a(x)g + g^{-1}dg.$$

Then the generic Berry phases satisfies, $\gamma_1(A_{\mathcal{R}}) \equiv \gamma_1(A)$ and $\gamma_3(a_{\mathcal{R}}) \equiv \gamma_3(a)$ in modulo 1. Here note that the γ_1 and γ_3 are defined by the integral over the odd dimensional spaces S^1 and S^3. Therefore the generic Berry phases γ_1 and γ_3 are *odd by the inversion/reflection of the parameter space S^2 and S^3, $x \to x_{\mathcal{I}}$ or $x \to x_{\mathcal{R}}$,* as

$\gamma_1(A_{\mathcal{I}}) = \gamma_1(A_{\mathcal{R}}) = -\gamma_1(A)$ and $\gamma_3(a_{\mathcal{I}}) = \gamma_3(a_{\mathcal{R}}) = -\gamma_3(a)$. Therefore we have a $\mathbb{Z}_2$-quantization of the Berry phases as

$$\gamma_1(A_{\mathcal{I}}) \equiv \gamma_1(A_{\mathcal{R}}) \equiv \gamma_1(A) = 0, 1/2 \pmod 1$$
$$\gamma_3(a_{\mathcal{I}}) \equiv \gamma_3(a_{\mathcal{R}}) \equiv \gamma_3(a) = 0, 1/2 \pmod 1$$

6.3. *Chiral symmetry for the minimum models*

The chiral symmetry of the minimum models discussed before are typical example of the systems with the inversion equivalence since the anti-commutators for the unitary $\Gamma = \Gamma^\dagger$ and $H_{\mathbb{C}}/H_{\mathbb{H}}$ are rewritten as

$$\Gamma^\dagger H_{\mathbb{C}}(\boldsymbol{R})\Gamma = -H_{\mathbb{C}}(\boldsymbol{R}) = H_{\mathbb{C}}(-\boldsymbol{R}) = H_{\mathbb{C}}(\boldsymbol{R}_{\mathcal{I}}),$$
$$\Gamma^\dagger H_{\mathbb{H}}(\boldsymbol{Q})\Gamma = -H_{\mathbb{H}}(\boldsymbol{Q}) = H_{\mathbb{H}}(-\boldsymbol{Q}) = H_{\mathbb{H}}(\boldsymbol{R}_{\mathcal{I}})$$

where the models are defined on the equators as $\boldsymbol{R} \in S^1$ and $\boldsymbol{Q} \in S^3$. This is what we need for the $\mathbb{Z}_2$-quantization of γ_1 and γ_3. We explicitly confirm it by direct calculations below.

Let us first consider a generic case without the KR degeneracy. In the north pole gauge, the multiplet at the equator $R_3 = 0$, $|z| = 1$ is given as $\Psi_N = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \bar{z} \end{bmatrix}$. Then we have $A_N = \frac{1}{2} z d\bar{z} = \frac{1}{2} g_{\mathbb{C}}^{-1} dg_{\mathbb{C}}$, $(g_{\mathbb{C}} = \bar{z} \in S^1)$. It implies $\gamma_1(A_N) = \frac{1}{2} W_{S^1}(g_{\mathbb{C}}) = -1/2$. If we take the south pole gauge, we have $\Psi_S = \frac{1}{\sqrt{2}}\begin{bmatrix} z \\ 1 \end{bmatrix}$, $A_S = \frac{1}{2}\bar{z}dz = -\frac{1}{2} z d\bar{z} = -A_N$, $(\bar{z}z = 1)$. It implies $\gamma_1(A_S) = +\frac{1}{2} \equiv \gamma_1(A_N)$, (mod 1). It is consistent with the general consideration and the $\mathbb{Z}_2$-quantization.

With the KR degeneracy, the connection is obtained just by replacing z to q. Then we have the Berry connections in the two gauges as $a_N = \frac{1}{2} q d\bar{q}$ and $a_S = \frac{1}{2}\bar{q}dq$. Note here that $a_S \neq -a_N$ which is different from the case without the KR degeneracy. Then using $dq = -qd\bar{q}q$ ($\bar{q}q = 1$, $d\bar{q}q = -\bar{q}dq$) and $da_N = \frac{1}{2} dq d\bar{q} = -\frac{1}{2} qd\bar{q}q \cdot d\bar{q} = -\frac{1}{2}(qd\bar{q})^2$, we have

$$\omega_3(a_N) = T(a_N da_N + \frac{2}{3} a_N^3) = T\big(-\frac{1}{4}(qd\bar{q})^3 + \frac{1}{12}(qd\bar{q})^3\big) = -\frac{1}{6} T(qd\bar{q})^3$$
$$\gamma_3(a_N) = \frac{1}{48\pi^2}\int_{S^3} T(g_{\mathbb{H}}^{-1} dg_{\mathbb{H}})^3 = \frac{1}{2} W_{S^3}(g_{\mathbb{H}}) = -\tfrac{1}{2}, \quad g_{\mathbb{H}} \in Sp(1).$$

Similarly we have $a_S = \frac{1}{2}\bar{q}dq = -\frac{1}{2}\bar{q}\cdot qd\bar{q}q = -\frac{1}{2} d\bar{q}q$, $da_S = \frac{1}{2} d\bar{q}dq = -\frac{1}{2} d\bar{q}\cdot qd\bar{q}q = -\frac{1}{2}(d\bar{q}q)^2$ and

$$\omega_3(a_S) = T(a_S da_S + \frac{2}{3} a_S^3) = T(\frac{1}{4}(d\bar{q}q)^3 - \frac{1}{12}(d\bar{q}q)^3\big) = \frac{1}{6} T(d\bar{q}q)^3 = \frac{1}{6} T(qd\bar{q})^3$$
$$\gamma_3(a_S) = -\gamma_3(a_N) = \tfrac{1}{2} \equiv \gamma_3(a_N) \mod 1$$

It again confirms the $\mathbb{Z}_2$-quantization of the quaternionic minimum model with the chiral symmetry.

6.4. *Reflection and TR invariant system without KR degeneracy*

The quantization of the $\mathbb{Z}_2$ Berry phase discussed in Sec.6.1 [13] can be considered as the quantization due to the reflection equivalence discussed in Sec.6.2 when the parameter introduced is the $U(1)$ twist e^{ix} and the other parameters are all real. It is simply due to the following observation of the TR invariance

$$\Theta^{-1} H(e^{ix})\Theta = U^\dagger H(e^{-ix})U = H(e^{ix})$$

where U is a unitary operator to change $c_{i\sigma} \to (-)^{(1-\sigma)/2} c_{i-\sigma}$ for the fermions and the spins $\boldsymbol{S}_i = \frac{1}{2}\boldsymbol{c}_i^\dagger \sigma \boldsymbol{c}_i$, $\boldsymbol{c}_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$. This is just the inversion or the reflection equivalence as discussed in Sec.6.2.

7. Topological Charge and nonlinear σ-models

Finally in this section, let us calculate topological charges of the nonlinear σ-model [49, 57, 58, 59, 60, 30] as applications of the gauge invariant forms of the Chern numbers C_1 and C_2 in Sec.4.

7.1. Topological charge without KR degeneracy [57, 58, 61]

Let us start by considering a parameter x dependent two component normalized state $\Psi(x) = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$, $\Psi^\dagger\Psi = 1 = |\mathrm{Re}\, z_1|^2 + |\mathrm{Im}\, z_1|^2 + |\mathrm{Re}\, z_2|^2 + |\mathrm{Im}\, z_2|^2$, which defines S^3. Then following 3 real quantities n_1, n_2, n_3 are defined as a CP^1 representation of n_i, $(i = 1, 2, 3\ )$

$$\boldsymbol{n}(x) = \begin{bmatrix} n^1 \\ n^2 \\ n^3 \end{bmatrix} = \Psi^\dagger \begin{bmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{bmatrix} \Psi = \begin{bmatrix} \Psi^\dagger\sigma^1\Psi \\ \Psi^\dagger\sigma^2\Psi \\ \Psi^\dagger\sigma^3\Psi \end{bmatrix} = \begin{bmatrix} \mathrm{Tr}_2\, \sigma^1 P \\ \mathrm{Tr}_2\, \sigma^2 P \\ \mathrm{Tr}_2\, \sigma^3 P \end{bmatrix}$$

where $\sigma_a = \sigma^a$ and the projection, $P(x) = \Psi\Psi^\dagger$, into the subspace spanned by $\Psi(x)$ is introduced.

Since $\mathrm{Tr}\, P = \Psi^\dagger\Psi = 1$, the projection is expanded as $P = \frac{1}{2}E_2 + P_i\sigma^i$. The coefficients are given as $P_i = \mathrm{Tr}\, P\frac{1}{2}\sigma^i = \frac{1}{2}n^i$. Now we have rewritten $P = \frac{1}{2}(E_2 + n_i\sigma^i) = \frac{1}{2}\big(E_2 + H_{\mathbb{C}}(\boldsymbol{n})\big)$ and $H_{\mathbb{C}} = \boldsymbol{n}\cdot\sigma = 2P - E_2$. Then $H_{\mathbb{C}}^2 = 4P - 4P + E_2 = E_2 = n_i\sigma_i n_j\sigma_j = n_i n_i + \sum_{i<j} n_i n_j\{\sigma_i, \sigma_j\} = |\boldsymbol{n}|^2 E_2$. It implies $|\boldsymbol{n}|^2 = 1$. Therefore the state Ψ can be considered as a positive energy eigen state of $H_{\mathbb{C}}$ by identifying $\boldsymbol{n} = \boldsymbol{R}$. It makes a CP^1 representation of the $SO(3)$ nonlinear σ-model.

Using this decomposition of the three vectors $\boldsymbol{n}$, let us discuss the topological charge of the current

$$J^\mu = \frac{1}{8\pi}\epsilon^{\mu\nu\lambda}\epsilon_{abc} n^a \partial_\nu n^b \partial_\lambda n^c$$

The topological charge is evaluated as

$$\begin{aligned} Q_{\mathbb{C}} &= \int dx^1 dx^2 J^3 = \frac{1}{8\pi}\int dx^1 dx^2 \epsilon^{3\nu\lambda}\epsilon_{abc} n^a\partial_\nu n^b \partial_\lambda n^c \\ &= \frac{1}{8\pi}\int dx^1 dx^2 \epsilon_{abc}(n^a\partial_1 n^b\partial_2 n^c - n^a\partial_2 n^b \partial_1 n^c) \\ &= \frac{1}{8\pi}\int \epsilon_{abc} n^a dn^b dn^c = \frac{1}{8\pi}\int \epsilon_{abc}(\mathrm{Tr}\,\sigma^a P)(\mathrm{Tr}\,\sigma^b dP)(\mathrm{Tr}\,\sigma^c dP) \end{aligned}$$

Since dP is traceless 2×2 hermite matrix as $0 = d1 = d\mathrm{Tr}\, P = \mathrm{Tr}\, dP$, we can expand dP and P as $dP = dP_a\sigma^a$, $P = \frac{1}{2}E_2 + P_a\sigma^a$, $(dP_a, P_a \in \mathbb{C},\ a = 1, 2, 3)$. Now we have

$$Q_{\mathbb{C}} = \frac{1}{8\pi}\int \epsilon_{abc} 2^3 P_a dP_b dP_c = \frac{1}{\pi}\int \epsilon_{abc} P_a dP_b dP_c$$

Also note that $\mathrm{Tr}\, PdPdP = P_a dP_b dP_c \,\mathrm{Tr}\, \sigma^a\sigma^b\sigma^c = P_a dP_b dP_c i\epsilon^{abd}\,\mathrm{Tr}\,\sigma_d\sigma^c = 2i\epsilon^{abc}P_a dP_b dP_c$. Therefore we finally have

$$C_1 = \frac{i}{2\pi}\int d\omega_1 = \frac{i}{2\pi}\int \mathrm{Tr}(PdPdP) = \frac{i}{2\pi}\int (2i)\epsilon_{abc}P_a dP_b dP_c = -Q_{\mathbb{C}}$$

It gives a direct relation between the first Chern number and the topological charge of the SO(3) nonlinear σ-model.

7.2. Topological charge with KR degeneracy [49, 57, 58, 59, 60, 30]

Similarly with the KR degeneracy, let us consider a x dependent four component normalized KR pair, which is described by the two component quaternionic vector $\psi(x) = \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} \in \mathbb{H}^2$, $\psi^\dagger\psi = 1 = (\psi_1^0)^2 + (\psi_1^1)^2 + (\psi_1^2)^2 + (\psi_1^3)^2 + (\psi_2^0)^2 + (\psi_2^1)^2 + (\psi_2^2)^2 + (\psi_2^3)^2$, which defines S^7 where $\mathbb{H} \ni \psi_i = \psi_i^0 + \psi_i^1 i_{\mathbb{H}} + \psi_i^2 j_{\mathbb{H}} + \psi_i^3 k_{\mathbb{H}}$, $\psi_i^a \in \mathbb{R}$, $(a = 0,1,2,3, i = 1,2)$. Then following 5 real quantities n_1, n_2, n_3, n_4, n_5 are defined by the HP^1 representation as

$$\boldsymbol{n}(x) = \begin{pmatrix} n^1\\ n^2\\ n^3\\ n^4\\ n^5\end{pmatrix} = \frac{1}{2}T\psi^\dagger \begin{pmatrix}\Sigma^1\\ \Sigma^2\\ \Sigma^3\\ \Sigma^2\\ \Sigma^5\end{pmatrix}\psi = \frac{1}{2}\begin{pmatrix} T\psi^\dagger\Sigma^1\psi\\ T\psi^\dagger\Sigma^2\psi\\ T\psi^\dagger\Sigma^3\psi\\ T\psi^\dagger\Sigma^4\psi\\ T\psi^\dagger\Sigma^5\psi\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\mathrm{Tr}\,T\,\Sigma^1 p\\ \mathrm{Tr}\,T\,\Sigma^2 p\\ \mathrm{Tr}\,T\,\Sigma^3 p\\ \mathrm{Tr}\,T\,\Sigma^4 p\\ \mathrm{Tr}\,T\,\Sigma^5 p\end{pmatrix},$$

$$\Sigma^1 = \begin{bmatrix} 0 & i_{\mathbb{H}}\\ \bar{i}_{\mathbb{H}} & 0\end{bmatrix}, \Sigma^2 = \begin{bmatrix} 0 & j_{\mathbb{H}}\\ \bar{j}_{\mathbb{H}} & 0\end{bmatrix}, \Sigma^3 = \begin{bmatrix} 0 & k_{\mathbb{H}}\\ \bar{k}_{\mathbb{H}} & 0\end{bmatrix}, \Sigma^4 = \begin{bmatrix} 0 & 1\\ 1 & 0\end{bmatrix}, \Sigma^5 = \begin{bmatrix} 1 & 0\\ 0 & -1\end{bmatrix}$$

where $\Sigma^a = \Sigma_a = (\Sigma^a)^\dagger$, $(\Sigma^a)^2 = E_2$, $\{\Sigma_a, \Sigma_b\} = 0$, $\Sigma^a\Sigma^b\Sigma^c\Sigma^d = \epsilon^{abcde}\Sigma_e$ (when a,b,c,d,e all different) and $p(x) = \psi\psi^\dagger$ is a projection, into the subspace spanned by the KR pair $\psi(x)$.

Since $\mathrm{Tr}\,T\,p = T\psi^\dagger\psi = 2$, the projection is expanded as $p = \frac{1}{2}E_2 + p_a\Sigma^a$. The coefficients are given as $p_a = \mathrm{Tr}\,T\,(\Sigma^a p)/4 = n^a/2$. Now we have rewritten $p = \frac{1}{2}(E_2 + n_a\Sigma^a) = \frac{1}{2}\big(E_2 + H_{\mathbb{H}}(\boldsymbol{n})\big)$ and $H_{\mathbb{H}} = \boldsymbol{n}\cdot\boldsymbol{\Sigma} = 2p - E_2$. Then $H_{\mathbb{H}}^2 = 4p - 4p + E_2 = E_2 = n_i\Sigma_i n_j\Sigma_j = n_i n_i E_2 + \sum_{i<j} n_i n_j\{\Sigma_i, \Sigma_j\} = |\boldsymbol{n}|^2 E_2$. It implies $|\boldsymbol{n}|^2 = 1$. Therefore the state ψ can be considered as a positive energy KR multiplet of $H_{\mathbb{H}}$ by identifying $\boldsymbol{n} = \boldsymbol{Q}$. It establishes the relation for the HP^1 representation of the $SO(5)$ nonlinear σ-model.

Again using this decomposition of the five vectors $\boldsymbol{n}$, let us discuss the topological charge $Q_{\mathbb{H}}$ following the references[59, 60, 30]

$$\begin{aligned} J^{\sigma\tau\omega} &= N^{-1}\epsilon^{\mu\nu\lambda\kappa\rho\sigma\tau\omega}\epsilon_{abcde}n^a\partial_\mu n^b\partial_\nu n^c\partial_\lambda n^d\partial_\rho n^e\\ Q_{\mathbb{H}} &= \int dx^1dx^2dx^3dx^4\, J^{567} = N^{-1}\int dx^1dx^2dx^3dx^4\,\epsilon^{\mu\nu\lambda\rho 567}\epsilon_{abcde}n^a\partial_\mu n^b\partial_\nu n^c\partial_\lambda n^d\partial_\rho n^e\\ &= N^{-1}\int \epsilon_{abcde}n^a dn^b dn^c dn^d dn^e\\ &= N^{-1}2^{-5}\int \epsilon_{abcde}(\mathrm{Tr}\,T\,\Sigma^a p)(\mathrm{Tr}\,T\,\Sigma^b dp)(\mathrm{Tr}\,T\,\Sigma^c dp)(\mathrm{Tr}\,T\,\Sigma^d dp)(\mathrm{Tr}\,T\,\Sigma^e dp)\end{aligned}$$

where N is a normalization constant.

Since dp is traceless quaternionic and hermite $0 = d1 = d\mathrm{Tr}\, p = \mathrm{Tr}\, dp$, we can expand dp and p as $dp = dp^a\Sigma_a$, $p = \frac{1}{2}E_2 + p^a\Sigma_a$, $(p^a, dp^a \in \mathbb{R}, a = 1,\cdots,5)$. Now

we have $Q_{\mathbb{H}} = 2^5 N^{-1} \int \epsilon_{abcde} p^a dp^b dp^c dp^d dp^e$. Also we can show $\mathrm{Tr}\, T\, (pdpdp)^2 = 4\epsilon_{abcde} p^a dp^b dp^c dp^d dp^e$. Therefore we have

$$C_2 = -\frac{1}{8\pi^2} \int \mathrm{Tr}\, T\, (pdpdp)^2 = -\frac{1}{2\pi^2} \int \epsilon_{abcde} p^a dp^b dp^c dp^d dp^e \propto Q_{\mathbb{H}}$$

This is again the direct relation between the second Chern number of the HP^1 model and the topological charge of the $SO(5)$ nonlinear σ-model.

8. Acknowledgments

We thank discussions with T. Fukui, H. Aoki, H. Katsura, M. Arai, I. Maruyama, M. Arikawa and T. Fujiwara about related materials. The work is supported in part by Grants-in-Aid for Scientific Research, No.20340098, No.20654034 from JSPS and No.220029004 (Physics of New Quantum Phases in Super-clean Materials) and No.20046002 (Novel States of Matter Induced by Frustration) on Priority Areas from MEXT (JAPAN). The work was also supported in part by the National Science Foundation under Grant No. PHY05-51164 at KITP (Santa Barbara) where a part of the work was done during the mini program "Quantum Spin Hall Effect and Topological Insulators".

References

[1] Dirac P A M 1931 *Proc. R. Soc.* **A 133** 60
[2] Thouless D J 1998 *Topological QUantum Numbers in Nonrelativistic Physics* (World Scientific)
[3] Thouless D J, Kohmoto M, Nightingale P and den Nijs M 1982 *Phys. Rev. Lett.* **49** 405
[4] Simon B 1983 *Phys. Rev. Lett.* **51** 2167
[5] Niu Q, Thouless D J and Wu Y S 1985 *Phys. Rev. B* **31** 3372
[6] Kohmoto M 1985 *Ann. Phys. (N. Y.)* **160** 355
[7] Hatsugai Y 1993 *Phys. Rev. Lett.* **71** 3697
[8] Berry M V 1984 *Proc. R. Soc.* **A392** 45
[9] Wen X G 1989 *Phys. Rev. B* **40** 7387
[10] Wen X G 1990 *Int. J. Mod. Phys. B* **4** 239
[11] Hatsugai Y 2004 *J. Phys. Soc. Jpn.* **73** 2604
[12] Hatsugai Y 2005 *J. Phys. Soc. Jpn.* **74** 1374
[13] Hatsugai Y 2006 *J. Phys. Soc. Jpn.* **75** 123601
[14] Hirano T, Katsura H and Hatsugai Y 2008 *Phys. Rev. B* **77** 094431
[15] Hirano T, Katsura H and Hatsugai Y 2008 *Phys. Rev. B* **78** 054431
[16] Maruyama I, Hirano T and Hatsugai Y 2009 *Phys. Rev. B* **79** 115107
[17] Arikawa M, Tanaya S, Maruyama I and Hatsugai Y 2009 *Phys. Rev. B* **79** 205107
[18] Halperin B I 1982 *Phys. Rev. B* **25** 2185
[19] Hatsugai Y 1993 *Phys. Rev. B* **48** 11851
[20] Hatsugai Y 1997 *J. Phys. C, Condens. Matter* **9** 2507
[21] Katsura H, Hirano T and Hatsugai Y 2007 *Phys. Rev. B* **76** 012401
[22] Hatsugai Y 2009 *Solid State Comm.* **149** 1016
[23] Wang Z, Chong Y D, Joannopoulos J D and Soljacic M 2008 *Phys. Rev. Lett.* **100** 013905
[24] Scarola V and Sarma S D 2007 *Phys. Rev. Lett.* **98** 210403
[25] Schnyder A P, Ryu S, Furusaki A, and Ludwig A W W 2008 *Phys. Rev. B* **78** 195125
[26] Kane C L and Mele E J 2005 *Phys. Rev. Lett.* **95** 146802
[27] Bernevig B A, Hughes T L and Zhang S C 2006 *Science* **314** 1757
[28] Qi X L, Hughes T L and Zhang S C 2008 *Phys. Rev. B* **78** 195424
[29] Avron J E, Sadun L, Segert J and Simon B 1989 *Phys. Rev. Lett.* **61** 1329
[30] Demler E and Zhang S C 1999 *Ann. Phys. (N.Y.)* **271** 83
[31] Murakami S, Nagaosa N and Zhang S C 2004 *Phys. Rev. B* **69** 214512
[32] Fu L and Kane C L 2006 *Phys. Rev. B* **74** 195312
[33] Fu L, Kane C L and Mele E J 2007 *Phys. Rev. Lett.* **98** 106803
[34] Fukui T and Hatsugai Y 2007 *Phys. Rev. B* **75** 121403

[35] Fukui T, Fujiwara T and Hatsugai Y 2008 *J. Phys. Soc. Jpn* **77** 123705
[36] Moore J E, Ran Y and Wen X G 2008 *Phys. Rev. Lett* **101** 186805
[37] Essin A M, Moore J E and Vanderbilt D 2009 *Phys. Rev. Lett* **102** 146805
[38] Ryu S 2009 *Phys. Rev. B* **79** 075124
[39] Schnyder A P, Ryu S and Ludwig A W 2009 *Phys. Rev. Lett.* **102** 196804
[40] Dyson F J 1962 *J. Math. Phys.* **3** 140
[41] Zumino B 1962 *J. Math. Phys.* **3** 1055
[42] Wilczek F and Zee A 1984 *Phys. Rev. Lett.* **52** 2111
[43] Eguchi T, Gilkey P B and Hanson A J 1980 *Phys. Rep.* **66** 213
[44] Zumino B 1991 *Current Algebra and Anomaly* (World Scientific) p 362
[45] Avron J E, Seiler R and Simon B 1983 *Phys. Rev. Lett.* **51** 51
[46] Avron J E, Sadun L, Segert J and Simon B 1989 *Commun. Math. Phys.* **124** 595
[47] Yang C N 1978 *J. Math. Phys.* **19** 320
[48] Minami M 1979 *Prog. Theor. Phys.* **62** 1128
[49] Minami M 1980 *Prog. Theor. Phys.* **63** 303
[50] Wu T T and Yang C N 1975 *Phys. Rev. D* **12** 3845
[51] Bertlmann R A 1996 *Anomalies in Quantum Field Theory* (Oxford Unic. Press)
[52] Hatsugai Y and Ryu S 2002 *Phys. Rev. B* **65** 212510
[53] Hatsugai Y, Fukui T and Aoki H 2007 *Euro. Phys. J. Spec. Top.* **148** 133
[54] Creutz M 2008 *JHEP* **0804:017**
[55] Nielsen H B and Ninomiya M 1981 *Nucl. Phys. B* **185** 20
[56] Xiao D, Shi J, Clougherty D P and Niu Q arXiv 0711.1855
[57] Wilczek F and Zee A 1983 *Phys. Rev. Lett.* **51** 2250
[58] Wu Y S and Zee A 1984 *Phys. Lett. B* **147** 325
[59] Wu Y S and Zee A 1988 *Phys. Lett. B* **207** 39
[60] de Azcarraga J A, Izquierdo J M and Zakrzewski W J 1991 *J. Math. Phys.* **33** 1272
[61] Wen X G and Zee A 1988 *Phys. Rev. Lett.* **61** 1025